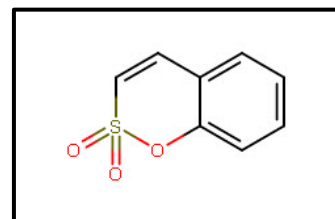


Substance Searching

I am interested in substituted sulfocoumarins (1,2-benzoxathiine-2,2-dioxides) and would also accept results comprising of fully or partly saturated analogues. I want any substituents on carbons in the sulfur-containing ring, and I want to allow for only one substituent on the other ring.



I'd then like to quickly analyze the results to see any relationships between functional groups and various properties.

In this workflow we show examples that include:

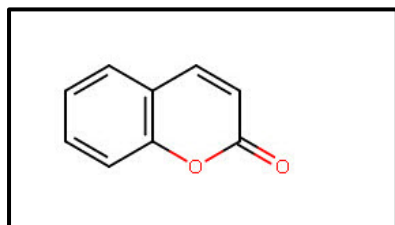
- How to create a structure template from a name
- How to make simple changes to the initial structure
- How to change the bond defaults
- How to attach a generic group at various points in the structure
- How to allow any substituent at selected points in the structure
- How to search for structures "As drawn"
- How to narrow initial answers so that they contain only those with specific functional groups

❖ Create a Structure Query

1. On the Reaxys home page click the **Create Structure or Reaction Drawing** box to open the structure editor (Marvin JS from ChemAxon).

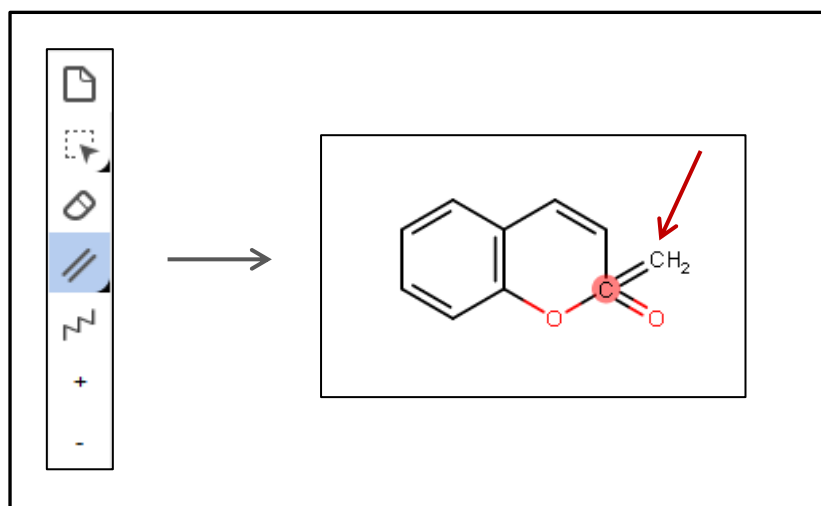


2. Draw or obtain the structure in the Marvin JS drawing panel:
 - a. Click **Create structure template from name**
 - b. Type **coumarin** and enter

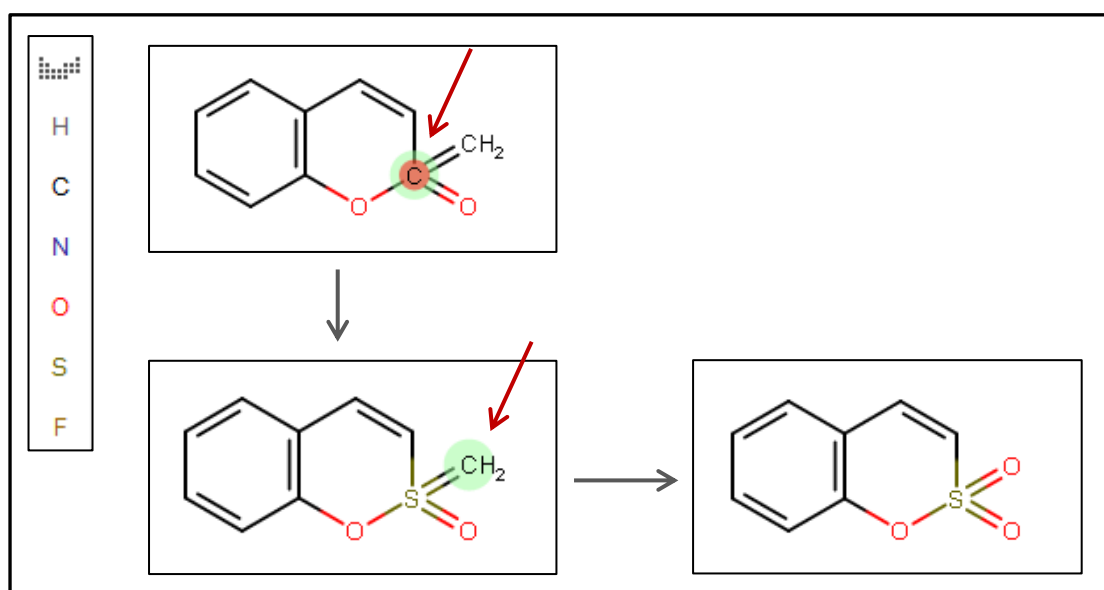


Edit the structure such that the **-O-CO-** group is replaced by **-O-SO₂-**.

3. Add a double bond:
 - a. Select the **Double bond** tool
 - b. Add a bond as shown



4. Change atoms as necessary:
 - a. Click '**S**' in the atom toolbar, click the '**C**' atom
 - b. Click '**O**' in the atom toolbar, click the '**CH₂**' atom



Edit the structure by adding 3 query features:

5. Add **Bond Properties**:

- Using the selection tool, select the bonds shown below (you can use the *Rectangle selection*, the *Freehand selection* (as shown below) or use the shift key to multi-select)
- Right click the selection and click **Bond properties**
- Click the **Type** drop down
- Click **any** and **Ok**

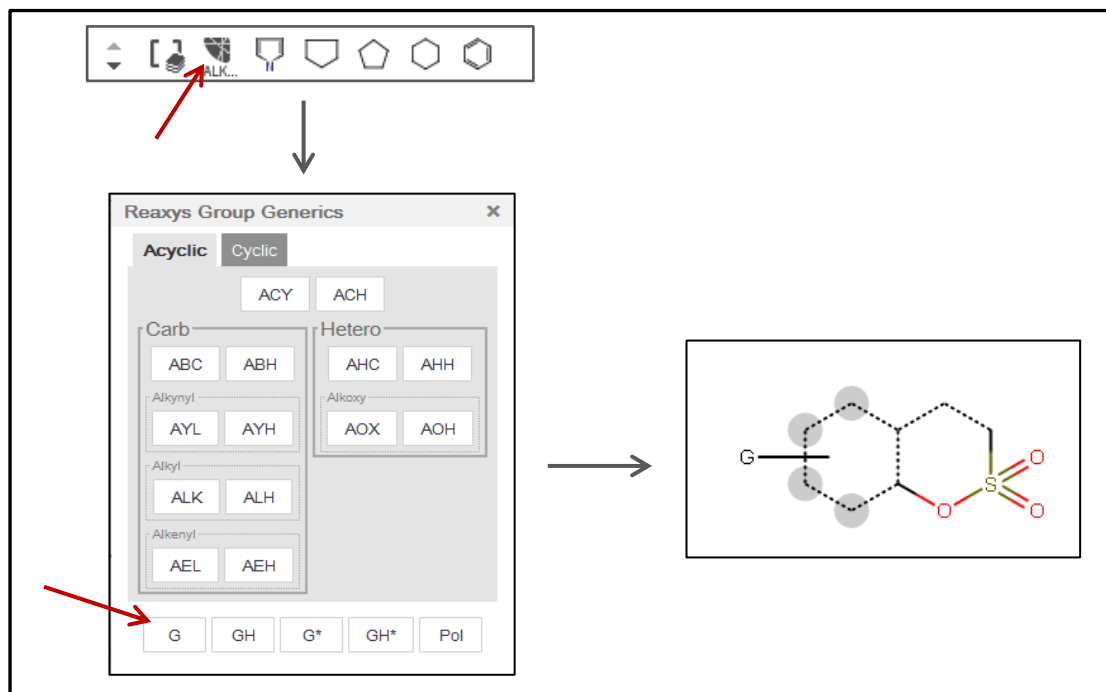
The diagram illustrates the process of adding bond properties to a chemical structure. It starts with a toolbar on the left containing a selection tool. The main structure shows a benzene ring and a sulfur-containing group (S=O) with a green freehand selection around them. A context menu is shown with 'Bond properties' selected. Below this, a 'Bond properties' dialog box is displayed with 'Type' set to 'any', 'Topology' set to 'undefined', and 'Reacting center' set to 'undefined'. An 'Ok' button is visible. The final structure shows the selected bonds with dashed lines, indicating the application of the 'any' bond property.

6. Add **Position variation bond**:

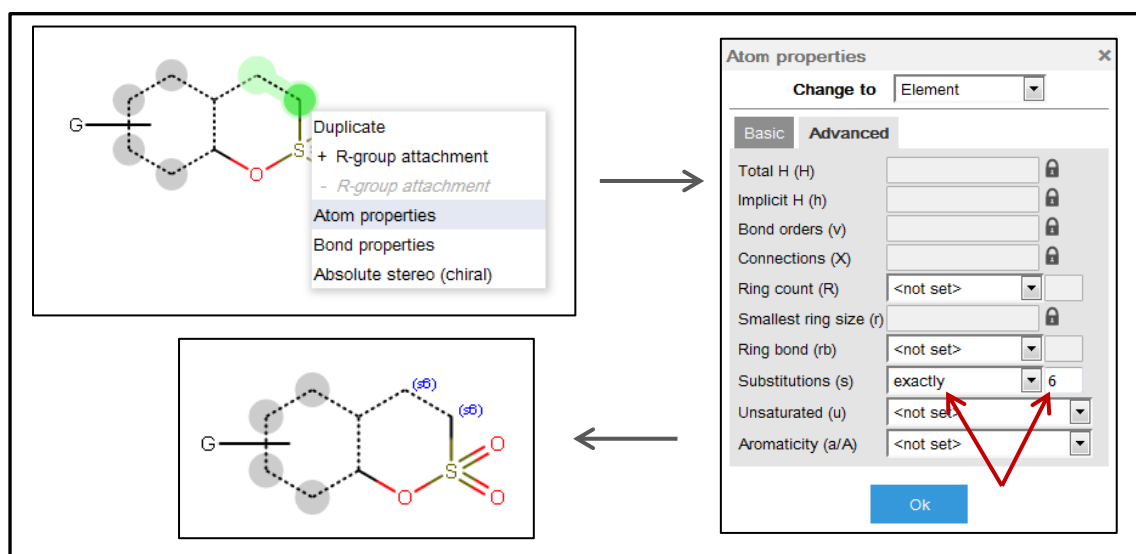
- Select the bonds shown below
- Click the **Position variation bond** tool from the toolbar

The diagram illustrates the process of adding a position variation bond to a chemical structure. It starts with a toolbar on the right containing various tools, with the 'Position variation bond' tool highlighted. The main structure shows a benzene ring and a sulfur-containing group (S=O) with a green selection around them. Below this, the final structure shows a methyl group (H₃C) attached to the benzene ring, indicating the application of the position variation bond.

7. Add the appropriate **Reaxys Generic Group (G)**:
 - a. Click the **ALK...** tool
 - b. In the **Acyclic** tab, click Any Group, in this case **G**
 - c. Click the end of the Position Variation Bond (**H₃C**) to change it to **G**



8. Allow **Substituents** in 2 locations by labeling the atoms below:
 - a. Press **Esc** on your keyboard to clear the previous tool selection
 - b. Select the two atoms shown
 - c. Right click the selection and click **Atom properties**
 - d. In the **Advanced** tab, click the **Substitutions(s)** drop down
 - e. Click **exactly** and set to **6**
 - f. Click **Ok**



The final query looks like this:

The screenshot shows the Reaxys 'Structure editor' with a chemical structure of a substituted benzothiazine derivative. The structure has a 'G' substituent on a benzene ring and two carbons in a fused ring system labeled 's6'. On the right, the 'Search this structure as:' panel is visible, with 'As drawn' selected. The 'Include' section has several options checked: Stereo, Additional ring closures, Salts, Mixtures, Isotopes, Charges, and Radicals.

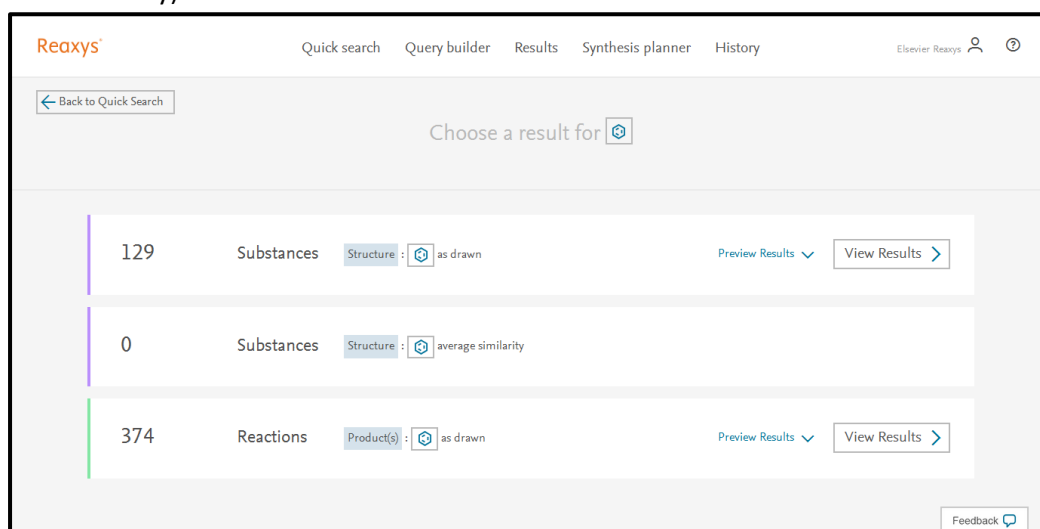
9. In the **Search this structure as:** panel, there are three options.
 - **As drawn:** Reaxys will find results for the query as drawn
 - **As substructure:** Reaxys offers two sub-options:
 - **On all atoms** will substitute any explicit or implicit hydrogen with any other atom or group
 - **On heteroatoms** will do the same but only on heteroatoms
 - **Similar:** Reaxys will find results for a similarity search based on the drawn query
- a. Click **As drawn** (the query already contains substructure search features that allow for a single substituent on the C6 ring, and any substituents on the two carbons marked (s6) shown in the other ring).
- b. In this example we are searching for the exact structure, therefore turn off all **Include** features

This screenshot is similar to the previous one but highlights the search options and include features. A red box surrounds the 'Search this structure as:' panel, and another red box surrounds the 'Include' section. Red arrows point from the 'As drawn' option to the 'Include' section, indicating that the 'As drawn' option is selected and the include features are being managed.

10. Click **Transfer to query** and click **Search**.

The Results Preview is displayed.

- Reaxys will present a Results Preview showing three different variations of the entered query to provide you with options, which you may not have thought of at query formulation time:
 - Exact Substance Results for the drawn query
 - Substance Results for a similarity search based on the drawn query (*Please note: the selected substructure attributes cannot be searched for similarity, which is the reason for 0 hits*)
 - Reaction Results for the drawn query (the structure will be searched as product automatically)

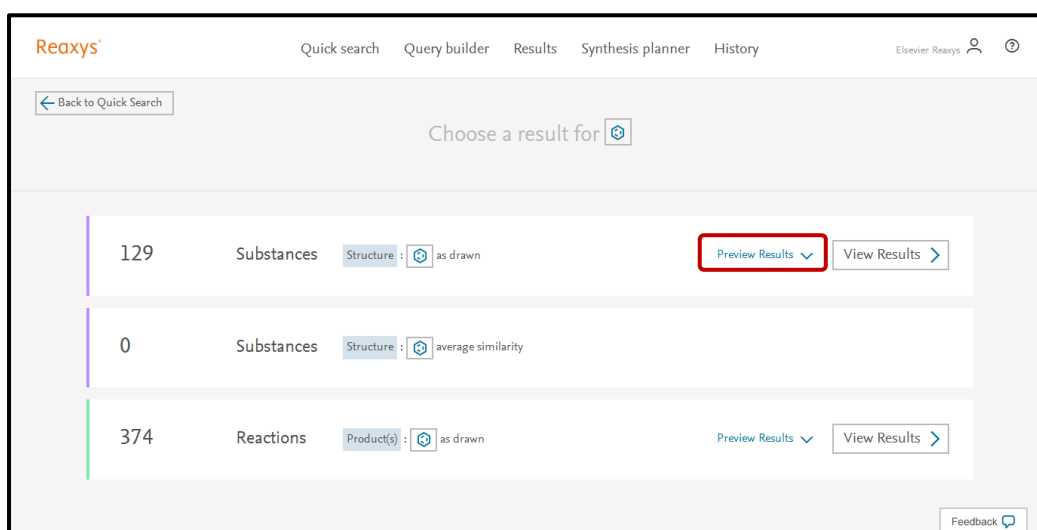


The screenshot displays the Reaxys search results preview interface. At the top, there is a navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. Below this, a 'Back to Quick Search' button is visible. The main content area is titled 'Choose a result for' and contains three search options:

- 129 Substances (Structure: as drawn) with a 'Preview Results' dropdown and a 'View Results' button.
- 0 Substances (Structure: average similarity) with a 'Preview Results' dropdown and a 'View Results' button.
- 374 Reactions (Product(s): as drawn) with a 'Preview Results' dropdown and a 'View Results' button.

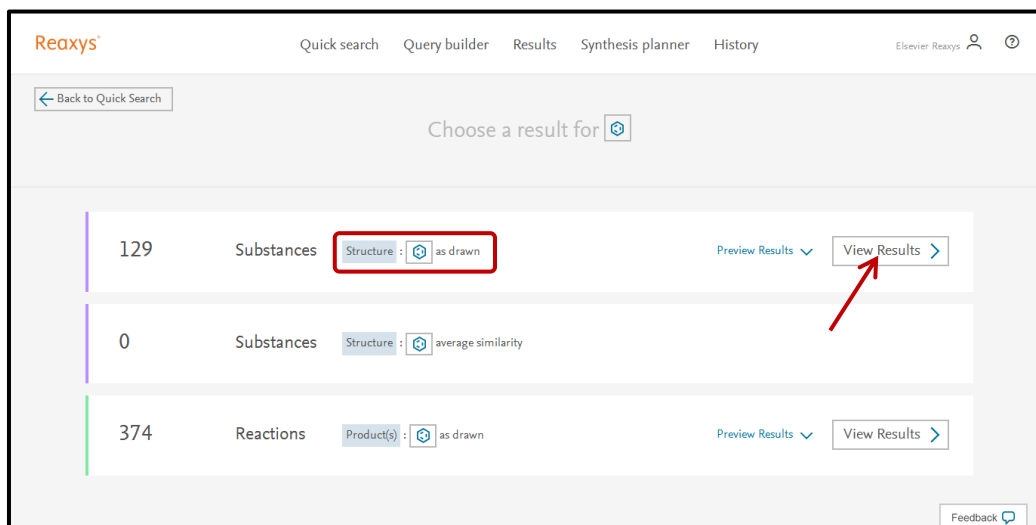
A 'Feedback' button is located at the bottom right of the interface.

- Each result set has a **Preview Results** feature that presents the top three results for the given query. You can check these top results before continuing to the full result set.



This screenshot is identical to the previous one, showing the Reaxys search results preview interface. The 'Preview Results' dropdown for the first search option (129 Substances) is highlighted with a red box, indicating that this feature is used to view the top three results for a given query before proceeding to the full result set.

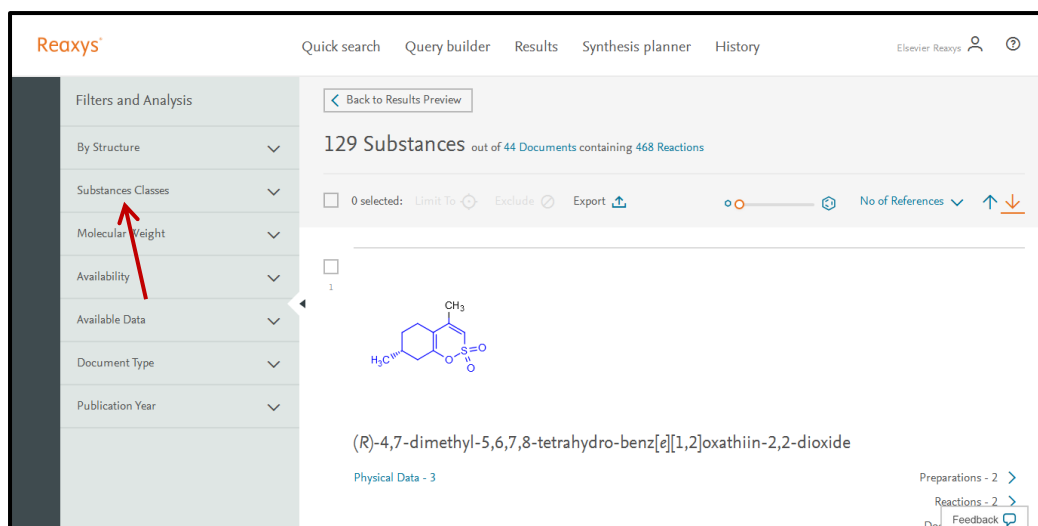
11. Click **View Results** for the first result set (Substances – as drawn).



❖ Analyze the Results

Use the *Filter & Analysis* panel to visualize information about these compounds. For example: I want to find out when articles on compounds with certain functional groups were published for the selected Alkyl Halides.

1. Compounds are classified into structural features that can be selected from the *Substance Classes*. The list presented in the filter panel is the first level of a hierarchically organized taxonomy.
 - a. Expand **Substances Classes**



- b. Click **+ More** to browse through the branches of the **Substance Classes** taxonomy.

Reaxys[®] Quick search Query builder Results Synthesis planner History Elsevier Reaxys

Filters and Analysis

By Structure

Substances Classes

- Functional Group Classification 128
- Richter Classification 128
- Ring Classification 128
- + More**
- Molecular Weight
- Availability
- Available Data
- Document Type

129 Substances out of 44 Documents containing 468 Reactions

0 selected: Limit To Exclude Export No of References

1

CN1CC2C(C)C(S(=O)(=O)O1)C2

(R)-4,7-dimethyl-5,6,7,8-tetrahydro-benz[e][1,2]oxathiin-2,2-dioxide

Physical Data - 3

Preparations - 2
Reactions - 2
DOI Feedback

- c. Click the text **Functional Group Classification**
- d. Check the box for **X in Functional Group** – to limit the results to halide compounds
- e. Click **Apply**

Clear selected

<input checked="" type="checkbox"/> Functional Group Classification 128	<input type="checkbox"/> O in Functional Group 128	<input checked="" type="checkbox"/> X
<input type="checkbox"/> Richter Classification 128	<input type="checkbox"/> S in Functional Group 128	<input type="checkbox"/> Br
<input type="checkbox"/> Ring Classification 128	<input type="checkbox"/> C=C in Functional Group 122	<input type="checkbox"/> Cl
	<input type="checkbox"/> N in Functional Group 54	<input type="checkbox"/> F
	<input checked="" type="checkbox"/> X in Functional Group 40	<input type="checkbox"/> I
	<input type="checkbox"/> C#C in Functional Group 1	

Apply

2. In the **Filters and Analysis** panel, expand the **Substance Classes** filter
 - a. Check the box for **Functional Group Classification** in the Substance Classes filter.

The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel on the left. Under 'Substances Classes', the 'Functional Group Classification' filter is checked and highlighted with a red arrow. The main results area shows 40 substances, with the first two being 6-bromo-1,2-benzoxathiine 2,2-dioxide and 6-iodo-1,2-benzoxathiine 2,2-dioxide. Each result includes a chemical structure, identification, and links to various data types like Preparations, Reactions, Spectra, and Documents.

- b. Scroll down and expand **Publication Year**

It shows us that most of the articles about this compound have been published in the last three to four years.

This screenshot shows the same search results as the previous one, but with the 'Publication Year' filter expanded in the 'Filters and Analysis' panel. The years 2011, 2013, 2016, and 2015 are highlighted with a red box, showing 13, 5, 4, and 4 substances respectively. The main results area remains the same, showing the chemical structures and associated data for the top two substances.

Please note: if you select an item in one filter then items in other filters will adapt accordingly (the number displayed represents the number of substances you will get, if you apply the filter selection).